Lunch Discussion: FASTMath Synergistic Activities
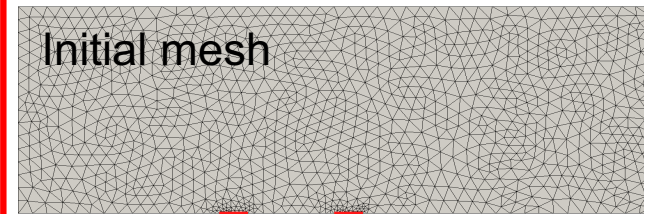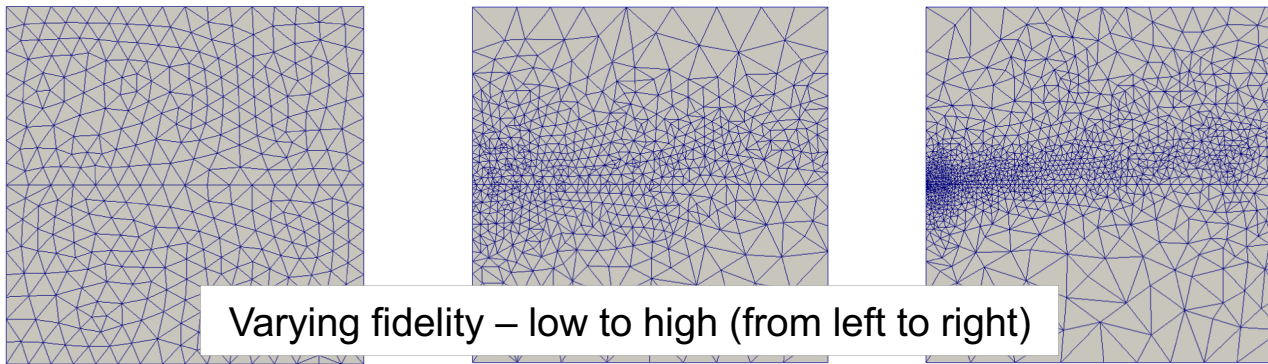
Moderated by: Carol Woodward

Synergistic activities in the FASTMath proposal

- Numerical optimization and uncertainty quantification (Habib Najm)
- Time integrators and linear solvers with numerical optimization and uncertainty quantification (Hong Zhang, poster, see slide)
- Unstructured mesh and uncertainty quantification (Onkar Sahni, poster, see slide)
- Data analytics and numerical optimization (Todd Munson, see slide)
- Data analytics and unstructured mesh (Rick Archibald)
- Time integrators and structured mesh (John Loffeld, poster)
- Linear solvers and structured mesh (Ulrike Yang, poster)
- Linear solvers and eigensolvers (Mathias Jacquelin, poster)
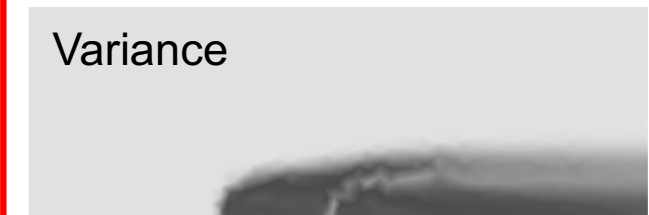- Software strategy (Ann Almgren, see RAPIDS session)

Unstructured Meshes in UQ Processes (Onkar Sahni, RPI)

- Unstructured meshes in UQ processes must address the following needs:
  - Reliable computation at UQ samples with control of mesh-based error
  - Multi-fidelity UQ employing multi-resolution meshes and models
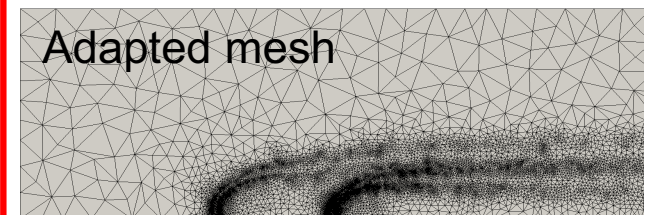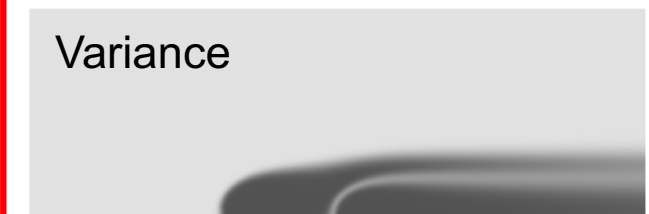 - Flexible stochastic representation of input and output data

Initial mesh

Jet 1   Jet 2

Variance

Jet 1   Jet 2

Adapted mesh

Jet 1   Jet 2

Variance

Jet 1   Jet 2

Multi-fidelity meshes (adaptively created)

Varying fidelity – low to high (from left to right)

FAST MATH

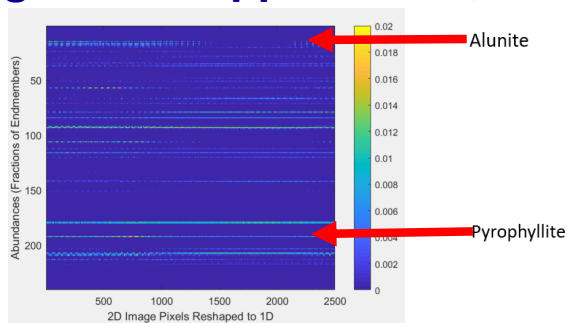# PETSc/TAO Optimization Solver with Joint-Sparsity Regularizer

- **Developed a solver for composite optimization with a smooth term and a non-smooth joint-sparse regularizer term**

$$\min_{\mathbf{L} \leq \mathbf{X} \leq \mathbf{U}} \frac{1}{2}\|\mathbf{AX} - \mathbf{B}\|_F^2 + \tau\|\mathbf{DX}\|_{2,1},$$

where $\mathbf{A} \in \mathbb{R}^{M \times N}$, $\mathbf{X} \in \mathbb{R}^{N \times L}$, $\mathbf{B} \in \mathbb{R}^{M \times L}$, $\mathbf{D} \in \mathbb{R}^{K \times N}$, $\tau > 0$,

$\|\mathbf{X}\|_F^2 := \sum_{i=1}^{N}\sum_{j=1}^{L}\mathbf{X}_{ij}^2$, and $\|\mathbf{X}\|_{2,1} := \sum_{i=1}^{N}\sqrt{\sum_{j=1}^{L}\mathbf{X}_{ij}^2}$.

  - **Construct a smooth approximation and apply the Gauss-Newton method**

  - **Provides flexibility to include joint sparsity with a dictionary transform and bounds**

  - **Available in next PETSc/TAO release**

- **Solver is scalable and suitable for large-scale joint-sparse regression applications, such as hyperspectral image un-mixing**
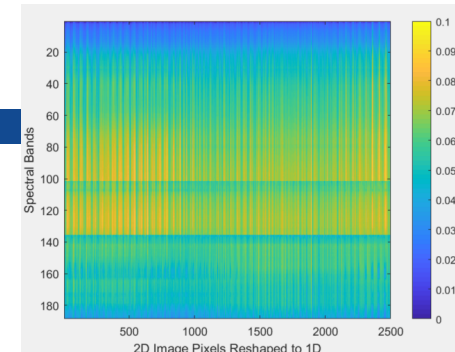

(a) Matrix B: 188 hyperspectral bands for 2500 image pixels

(b) Matrix A: 188 hyperspectral bands of 240 "minerals"

(c) Computed X: fractions of 240 "minerals" for 2500 image pixels
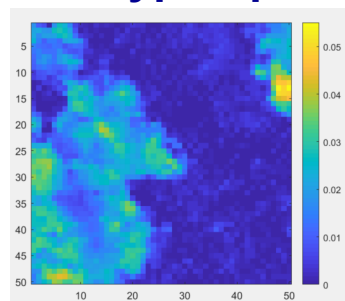
(d) Alunite component
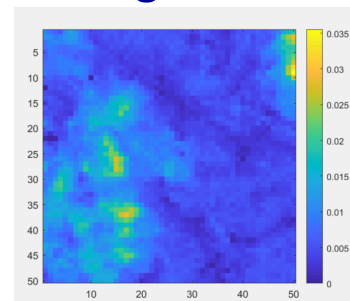
(e) Pyrophyllite component

Figure: Joint-sparsity reconstruction for hyperspectral un-mixing. (a) Cuprite sample, 188 spectral bands and 50x50 image pixels. (b) 240 pure spectral signatures. (c) Solution. (d) & (e) Alunite and Pyrophyllite reconstructions.

Xiang Huang, Alp Dener, and Todd Munson (ANL)

Discrete Adjoint Time-domain Sensitivity Analysis Capability in PETSc

- Calculating gradients is difficult and computationally expensive for PDEs

- We have developed first-order and second-order discrete adjoint sensitivity analysis capability that can
  - Avoid full differentiation of the code (traditional AD)
  - Avoid deriving the adjoint PDE (continuous adjoint)

- We have been working with the optimization team to use adjoint to efficiently solve PDE-constrained optimization problems

Hong Zhang, Argonne National Laboratory
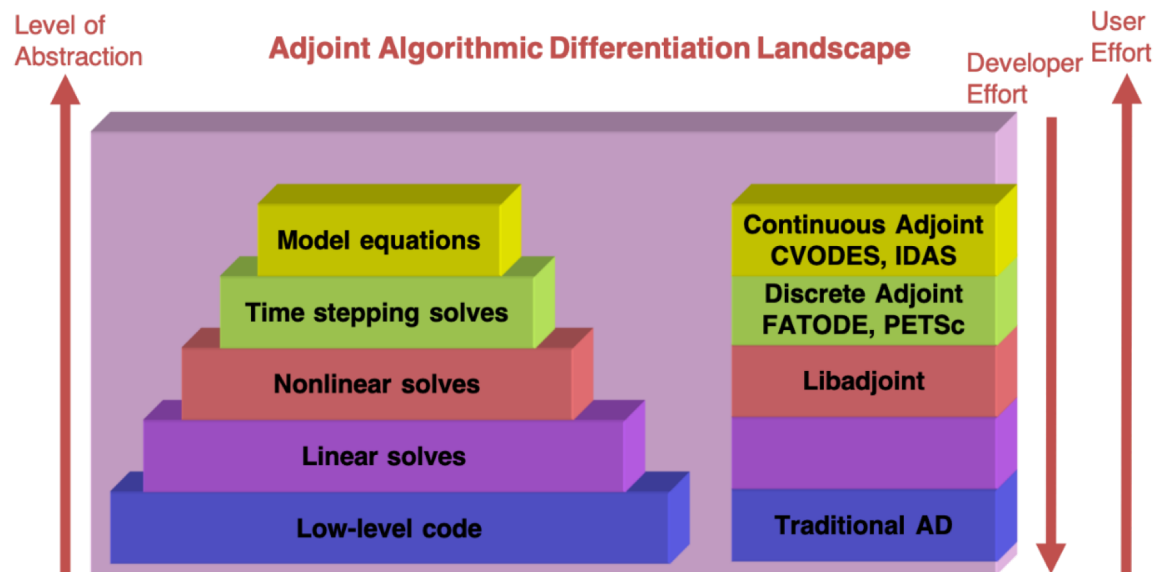
What synergistic activities are ongoing?

- What other synergistic activities are we pursuing?
- What are "best practices" that enabled synergistic activities?

What opportunities for further synergistic activities exist?

- What do people need from other parts of the FASTMath institute (e.g., "help! I need an eigensolver")?
- What are road-blocks to synergistic activities and how can we address them?